CORE-CM SEMINAR
Michigan State University — Department of Chemistry

Prof. Michael Wasielewski
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Exciton Dynamics and Structural Investigations of Singlet Fission in Molecular Solids

Singlet fission (SF) is the process by which a singlet exciton in a molecular material is energetically down-converted into two independent triplet excitons. Thermodynamic modeling predicts that using a SF material in a single-junction solar cell can theoretically increase the Shockley-Queisser limit for power conversion efficiency from 32% to 44%, assuming that SF results in the formation of two triplet excitons, each of which produce an electron-hole pair quantitatively. We are examining new dye molecules, which undergo SF, using guidance from electronic structure calculations to assure the requisite relationships between molecular singlet and triplet energy levels. We are preparing hierarchical assemblies from these chromophores, starting from covalent dimers and trimers, then developing supramolecular assemblies, and engineered crystalline materials to investigate SF in bulk, ordered materials. We are using femtosecond transient spectroscopy as well as time-resolved electron paramagnetic resonance spectroscopy to characterize the SF mechanism and the factors that determine its efficiency at time scales down to 100 fs. We are also using X-ray diffraction to investigate the single crystal structures of these materials and X-ray scattering on their thin polycrystalline solid films to determine how their structures correlate with their ability to carry out SF. Our results suggest that a π-π slip-stacked geometry is important for maximizing SF efficiency.

Thursday, February 27, 2014
12:00 PM
Room 1400 – BPS
Professor Jim McCusker – Host

Accommodations for persons with disabilities may be requested by calling the Chemistry Department at (517) 355-9715, X345 two days prior to the event to ensure sufficient time to make arrangements. Requests received after this date will be met when possible.